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(FILE 'HOME' ENTERED AT 16:26:14 ON 30 MAR 2007)

FILE 'CA' ENTERED AT 16:26:52 ON 30 MAR 2007

L1 5649 S (MS MS OR MASS SPECTRO?) AND ION TRAP?  
L2 704 S L1 AND (CID OR COLLISION(3A)DISSOCIAT?)  
L3 61 S L2 AND (DIOXIN OR CHLOR? OR CHLORIN?)  
L4 16 S L2 AND (POLYCHLOR? OR HALOGEN? OR POLYHALOGEN?)  
L5 24 S L2 AND (END CAP OR ENDCAP)  
L6 22 S L2 AND (ION (2A)CLEAV? OR TICKLE OR ALTERNATING CURRENT)  
L7 108 S L2 AND (FREQUENCY OR MULTIFREQUENCY OR EXCIT?)  
L8 69 S L3-7 AND PY<2000  
L9 7 S L3-7 NOT L8 AND PATENT/DT AND PY<2004  
L10 76 S L8-9

=> d bib,ab 1-76

L10 ANSWER 7 OF 76 CA COPYRIGHT 2007 ACS on STN

AN 132:315608 CA

TI Method of ion fragmentation in a quadrupole ion trap

IN Schwartz, Jae C.; Taylor, Dennis M.

PA Finnigan Corp., USA

SO PCT Int. Appl., 27 pp.

PI WO 2000024037 A1 20000427 WO 1999-US24188 19991014  
US 6124591 A 20000926 US 1999-416128 19991012

PRAI US 1998-104458P P 19981016  
US 1999-416128 A 19991012

AB Methods of generating product ions in a quadrupole ion trap are described which entail trapping ions having a mass-to-charge ratio of interest in the trap and exciting the ions by applying an excitation voltage selected to have an amplitude which is substantially linearly related to the mass-to-charge ratio of the selected ions to cause the selected ions to become kinetically excited and to collisionally dissociate. Methods of mass anal. employing the methods of ion fragmentation are also described.

L10 ANSWER 26 OF 76 CA COPYRIGHT 2007 ACS on STN

AN 128:217559 CA

TI Collision-Induced Signal Enhancement: A Method To Increase Product Ion Intensities in MS/MS and MS<sub>n</sub> Experiments

AU Asam, Michael R.; Ray, Kenneth L.; Glish, Gary L.

CS Department of Chemistry, University of North Carolina, Chapel Hill, NC, 27599, USA

SO Analytical Chemistry (1998), 70(9), 1831-1837

AB Collision-induced signal enhancement (CISE), a new technique to enhance the MS<sub>n</sub> capabilities of the quadrupole ion trap, is demonstrated. CISE is based on the chem., i.e., the dissociation pathways, of the analyte examined. Polysaccharides up to hexamers are used to demonstrate the capabilities of CISE to enhance signal in two distinct functional modes. Mode 1 CISE is designed to enhance the signal of an ion desired for MS<sub>n</sub> anal. Mode 2 CISE is designed to enhance structurally significant product ions in an MS/MS spectrum. Two different approaches can be utilized to effect the two functional modes of CISE. Both approaches

use conventional resonant **excitation** techniques to effect dissocn., which is performed non-anal., i.e., without isolation of the ions to be dissocd. The two approaches are (1) **single-frequency** resonance **excitation**, and (2) broad-band wave form resonant **excitation**. Exptl. results for Mode 1 CISE anal. demonstrate up to a 17.3-fold signal increase for the **single-frequency** approach and 5.3-fold using broad-band **excitation**. Mode 2 CISE anal. shows up to a 16.3-fold increase in signal strength with **single-frequency** **excitation** and 3.3-fold using broad-band **excitation**.

L10 ANSWER 27 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 128:192310 CA  
TI Collision-induced **dissociation** (CID) processes in some carbamate and phenylurea pesticides studied by **ion-trap MS/MS**  
AU Yinon, Jehuda; Vincze, Adam  
CS Department of Environmental Sciences and Energy Research, Weizmann Institute of Science, Rehovot, 76100, Israel  
SO International Journal of Mass Spectrometry and Ion Processes (1997), 167/168, 21-33  
AB A series of carbamate and phenylurea pesticides was studied by **ion-trap MS/MS** collision-induced **dissocn.** (CID) in the resonant **excitation** mode. CID mass spectra contained highly abundant daughter ions formed by simple cleavage as well as by rearrangement processes. The formation of rearrangement daughter **ions** vs. **cleavage** daughter **ions** was found to be dependent on the CID voltage and CID time in some of the investigated compds. The relative intensity of the **ions** formed by **cleavage**, i.e. via high-energy pathways, vs. ions formed through rearrangement processes, i.e. via low-energy pathways, increased with increasing collision energy. A similar effect was obtained by increasing the CID time, thus enabling the **ions** to gain more energy and consequently form more **cleavage** **ions** than rearrangement **ions**.

L10 ANSWER 28 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 128:110163 CA  
TI Tandem mass spectrometric determination of polychlorodibenzo-p-dioxins and polychlorodibenzofurans in a quadrupole ion trap using multi-frequency resonant **excitation**  
AU Splendore, Maurizio; Plomley, Jeffry B.; March, Raymond E.; Mercer, Roger S.  
CS Dep. Chem., Trent Univ., Peterborough, ON, K9J 7B8, Can.  
SO International Journal of Mass Spectrometry and Ion Processes (1997), 165/166, 595-609  
AB A tandem mass spectrometric anal. method is presented for the concurrent detn. of tetra- to octachlorodibenzo-p-dioxins and tetra- to octachlorodibenzofurans. The method entails operation of a quadrupole **ion trap mass spectrometer** wherein two isolated mol. ion species are fragmented by irradn. with a band of multiple **frequencies** for a period of but 10 ms. Up to three co-eluting compds. have been detd. individually using a software program, Toolkit, which permits successive activation of multiple scan functions customized for each compd. and optimized for the resonant **excitation** conditions employed. Two calibration curves have been obtained for each compd. over a 400-fold

concn. range; one calibration curve is based on the single major fragmentation channel of  $\text{COCl}^+$  loss, while the other is based on multiple fragmentation channels. The CID efficiency, defined as the signal ratio of fragment ions detected from the major dissociation channels to mol. ions isolated, was 0.80-0.90 for all **chloro** congeners. The calibration curves were prepd. using a set of std. solns. contg. labeled **chloro** congeners. Optimum results were obtained when fragment ion signal intensities were normalized to those obtained from a single std. soln. In general, tandem **mass spectrometric** response factors display a 4-fold range, with response factor decreasing with increasing **chlorine** substitution. octachlorodibenzofuran octachlorodibenzodioxin.

L10 ANSWER 29 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 128:86115 CA  
TI Development of a capillary high-performance liquid chromatography tandem **mass spectrometry** system using swift technology in an **ion trap**/reflectron time-of-flight **mass spectrometer**  
AU He, Ling; Wu, Jing-Tao; Parus, Steve; Lubman, David M.  
CS Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109-1055, USA  
SO Rapid Communications in Mass Spectrometry (1997), 11(16), 1739-1748  
AB In this work a capillary HPLC/tandem **mass spectrometry** system has been developed in a quadrupole **ion trap**/reflectron time-of-flight **mass spectrometer**. The broadband **excitation** for isolating a precursor ion is achieved by generating the stored waveform inverse Fourier transform waveform in real time. Following the isolation and cooling periods, an auxiliary AC voltage (**tickler**) is applied to the entrance **end cap** of the **ion trap** to generate **collision induced dissociation**. The amplitude of the **tickler** voltage is optimized online using a feedback method which involves having two computers communicating with each other. This system has been tested with a peptide mixt. and tandem mass spectra were obtained for each peptide.

L10 ANSWER 30 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 128:3875 CA  
TI Boundary-Activated Dissociation of Peptide Ions in a Quadrupole Ion Trap  
AU Vachet, Richard W.; Glish, Gary L.  
CS Department of Chemistry, University of North Carolina, Chapel Hill, NC, 27599, USA  
SO Analytical Chemistry (1998), 70(2), 340-346  
AB Boundary-activated dissociation (BAD) of peptides has been investigated as an alternative to the use of resonant **excitation** to effect **collision-induced dissociation** in the quadrupole **ion trap**. BAD's nonresonant **excitation** mechanism overcomes a major drawback in resonant **excitation**, namely, the variation of the resonant **excitation frequency** as a function of ion space charging. As with resonant **excitation**, the pulsed introduction of heavy gases (argon, xenon) extends the applicability of BAD when tandem **mass spectrometry** is performed on peptide ions. The presence of heavy gases during ion activation allows greater internal energy deposition and also enables BAD to be performed at much lower trapping field strengths (lower  $qz$  values) than previously reported for this technique. This extends the mass range over which product ions can

be collected.

L10 ANSWER 36 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 126:112562 CA  
TI Modulated resonant **excitation** of selected polychlorobiphenyl molecular ions in an **ion trap mass spectrometer**  
AU Lausevic, Mila; Splendore, Maurizio; March, Raymond E.  
CS Department of Chemistry, Trent University, Peterborough, ON, K9J 7B8, Can.  
SO Journal of Mass Spectrometry (1996), 31(11), 1244-1252  
AB Modulated resonant **excitation** leading to collisionally induced dissocn. (CID) of isolated mol. ions of di-ortho, mono-ortho and nonortho-substituted tetrachlorobiphenyl (PCB) compds. was accomplished in a quadrupole **ion trap**. While the **ion trap** was irradiated with a supplementary a.c. signal of fixed frequency, the r.f. drive voltage amplitude was modulated so as to sweep the ion absorption window. Modulated resonant **excitation** of PCB mol. ions was carried out over a wide range of exptl. conditions and congeners to compare the relative stabilities of such ions and their fragmentation behavior. Significant differences in both mol. ion stability and fragmentation patterns were obsd. for mono-ortho and nonortho-substituted tetrachlorobiphenyls compared with di-ortho-isomers. Based on the differences in fragmentation patterns obsd. in **CID** mass spectra, an anal. protocol is proposed for the ready detn. of the toxic mono-ortho- and nonortho-substituted PCB congeners in mixt. of PCBs. The protocol is based on the fragmentation behavior of mol. ions, and is illustrated with a mixt. of 13 PCB congeners.

L10 ANSWER 39 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 125:153623 CA  
TI Application of nonresonance **excitation** to **ion trap tandem mass spectrometry** and selected ejection chemical ionization  
AU Wang, Mingda; Schachterle, Steve; Wells, Greg  
CS Varian Chromatography Systems, Walnut Creek, CA, 94598, USA  
SO Journal of the American Society for Mass Spectrometry (1996), 7(7), 668-676  
AB Nonresonance **excitation** is a universal ion **excitation** and ejection method in which increased ion kinetic energy is achieved by the combination of an axial d.c. dipole and the radiofrequency trapping fields. The method does not require the applied **excitation frequency** to match with the secular **frequency** of the precursor ions to effect **collision-induced dissocn.** (CID) for **tandem mass spectrometry** applications. Therefore, it is free of the effects of secular **frequency** changes caused by space-charge and simplifies the optimization of **tandem mass spectrometry** parameters when combined with gas chromatog.-tandem **mass spectrometry** (GC-MS/MS). Computer simulations show that in contrast to the resonance **excitation** process, the nonresonance **excitation** process is able to accelerate thermal ions to kinetic energies >40 eV in a few microseconds. Based on simulations, the authors expect that the rapid deposition of energy by this method may allow the study, in **ion traps**, of high energy decompr. channels of precursor ions with multiple decompr. channels. Also, the method is

able to simultaneously **excite** multiple precursor ions, for example, **excite** both analyte and its coeluting isotopically labeled internal std. for GC-**MS/MS** anal. A GC-**MS/MS** anal. of 100 pg of n-butylbenzene is demonstrated with a signal-to-noise ratio of 3624, which is over in order of magnitude higher than the signal-to-noise ratio of 345 obtained by full scan gas chromatog.-**mass spectrometry**. The nonresonance **excitation** method can be used as a low pass mass filter in the chem. ionization (CI) mode to eject undesired fragment ions that result from direct electron ionization. This new CI method, selected ejection chem. ionization, can produce a CI spectrum without contamination of sample fragment ions from electron ionization.

L10 ANSWER 42 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 125:25295 CA  
TI Tandem **Mass Spectrometry** of **Polychlorodibenzo-p-Dioxin** and **Polychlorodibenzofuran** in a **Quadrupole Ion Trap**. 1. Comparison of **Single-Frequency**, **Secular Frequency** Modulation, and **Multifrequency** Resonant **Excitation** Modes  
AU Plomley, Jeffry B.; March, Raymond E.; Mercer, Roger S.  
CS Department of Chemistry, Trent University, Peterborough, ON, K9J 7B8, Can.  
SO Analytical Chemistry (1996), 68(14), 2345-2352  
AB A study was carried out on three modes of resonant **excitation** in the development of an anal. protocol for the detn. of **polychlorodibenzo-p-dioxins** (PCDDs) and **polychlorodibenzofurans** (PCDFs) by **ion trap tandem mass spectrometry**. The resonant **excitation** modes studied are **single-frequency** irradn. (SFI), **secular frequency** modulation (SFM), and **multifrequency** irradn. (MFI) of isolated mol. ion species. Each **excitation** mode was examd. for fragmentation channel selectivity so as to optimize instrument sensitivity. **Collision-activated dissociation** mass spectra obtained with each **excitation** mode are compared with those obtained by triple-stage quadrupole **mass spectrometry** (TSQMS). While the same reaction channels (corresponding to losses of Cl<sup>•</sup>, COCl<sup>•</sup>, and 2COCl<sup>•</sup> for PCDDs and Cl<sup>•</sup>, COCl<sup>•</sup>, and COCl<sub>2</sub> and COCl<sub>3</sub><sup>•</sup> for PCDFs) were obsd. for each **excitation** mode, the fragment ion relative abundances differed among the resonant **excitation** modes and showed that internal energy deposition in the precursor ion was in the order MFI > SFI > SFM. In each resonant **excitation** mode, the obsd. conversion efficiency for loss of COCl<sup>•</sup> exceeded that obsd. with TSQMS. The procedure of tuning SFI to ion secular **frequencies** was laborious, while the required duration of irradn. with SFM was excessively long compared to the gas chromatog. time scale. The tuning requirements of MFI using 1 and 2 kHz bandwidth pulses were less rigorous than those for SFI, and the duration of irradn. was compatible with the gas chromatog. time scale.

L10 ANSWER 51 OF 76 CA COPYRIGHT 2007 ACS on STN  
AN 123:241393 CA  
TI MS<sub>n</sub> techniques employing **collision-induced dissociation**  
IN Wells, Gregory J.; Wang, Mingda  
PA Varian Associates, Inc., USA; Varian Inc.  
SO Jpn. Kokai Tokkyo Koho, 8 pp.

PI JP 07169439 A 19950704 JP 1994-246747 19940916  
EP 643415 A2 19950315 EP 1994-306779 19940914  
PRAI US 1993-121844 A 19930915

AB MSn **mass spectrometric** techniques and methods for producing **collision-induced dissociation** of ions in quadrupole **ion traps** are described which entail scanning the trap potential through levels corresponding to the secular **frequencies** of the parent or daughter ions, as appropriate.

L10 ANSWER 55 OF 76 CA COPYRIGHT 2007 ACS on STN

AN 122:150604 CA

TI Methods of using **ion trap mass spectrometers**

IN Wells, Gregory J.; Wang, Minada

PA Varian Associates, Inc., USA

SO U.S., 21 pp. Cont.-in-part of U.S. Ser. No. 890,991, abandoned.

PI US 5381006 A 19950110 US 1993-43240 19930406

PRAI US 1992-890991 B2 19920529

AB Improved methods of using an **ion trap mass spectrometer**, whereby a.c. voltages supplemental to the a.c. trapping voltage were used for scanning the trap, for conducting chem. ionization expts., and for conducting MSn expts., are shown. In one embodiment a broadband supplemental a.c. voltage is applied to rid the trap of ions above or below a preselected cutoff mass. This is particularly useful in conducting chem. ionization expts. for eliminating high mass sample ions that are formed when the reagent gas is ionized by electron impact ionization. Likewise, this technique may be used to eliminate low mass reagent ions when conducting an electron impact ionization expt. in the presence of a reagent gas. In another embodiment a nonresonant, low-**frequency** supplemental voltage is applied to the trap causing trapped ions to undergo **collision induced dissociation**. Multiple generations of ion fragments may be simultaneously formed in this manner, thereby enabling MSn expts. The **low-frequency** supplemental field has the addnl. property of causing high mass ions to be ejected from the trap as a function of the magnitude of the supplemental voltage. This property may be used to scan the trap, for example, by scanning the magnitude of the supplemental voltage. Likewise, when conducting chem. ionization expts., this property may be used for eliminating unwanted high mass sample ions, formed during ionization of the reagent gas, from the trap.

L10 ANSWER 61 OF 76 CA COPYRIGHT 2007 ACS on STN

AN 119:17363 CA

TI Broad-band **excitation** in the quadrupole **ion trap mass spectrometer** using shaped pulses created with the inverse Fourier transform

AU Julian, Randall K., Jr.; Cooks, R. Graham

CS Dep. Chem., Purdue Univ., West Lafayette, IN, 47907, USA

SO Analytical Chemistry (1993), 65(14), 1827-33

AB Broad-band **excitation** is reported of ions in the quadrupole **ion trap mass spectrometer** (ITMS) using shaped pulses. In place of a single-**frequency excitation** signal, applied to the **end caps** of the ITMS, a shaped pulse which **excites** a broad spectrum of **frequencies** is used. Shaped pulses are time domain signals created by taking the complex inverse Fourier transform of a **frequency** domain function whose magnitude represents the desired **excitation** spectrum. In **mass spectrometry** these signals are termed SWIFT (stored wave form inverse Fourier transform)

pulses. By selection of a **frequency** spectrum which includes ion secular **frequencies**, SWIFT pulses can be constructed to **excite** a wide range of *m/z* values in the quadrupole **ion trap**. Using the phase modulation method described by Chen et al., the **frequency** domain spectrum is converted to a complex function prior to being transformed to the time domain. The time domain signal is then processed and loaded into an arbitrary wave form generator (ARB) connected to the **end-cap** electrodes and applied in a dipolar fashion. Three basic applications of SWIFT pulses are demonstrated in the quadrupole **ion trap**: (i) broad-band ejection of desorbed matrix ions by application of SWIFT pulses during ion injection from an external source, (ii) broad-band ejection of trapped ions for selective ion isolation, (iii) broad-band **excitation** which results in **collision-induced dissociation** (CID) of selected ions. Applying SWIFT pulses while ions are being injected from a Cs<sup>+</sup> desorption source results in ejection of matrix ions, which reduces space charge and greatly improves parent ion intensity and overall sensitivity. SWIFT pulses are effective at ejecting ions which have been stored for ion isolation, and the method shows good mass discrimination.

**L10 ANSWER 62 OF 76** CA COPYRIGHT 2007 ACS on STN

AN 118:265778 CA

TI Gas chromatography-tandem **mass spectrometry** implemented on a bench-top quadrupole **ion trap**-based instrument using random noise to effect **collision-induced dissociation**

AU Van Berkel, Gary J.; Goeringer, Douglas E.

CS Analytical Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

SO *Analytica Chimica Acta* (1993), 277(1), 41-54

AB A simple and effective method for **collision-induced dissociation** (CID), implemented through application of random noise to an **end-cap** electrode, allows gas chromatog. (GC)-tandem **mass spectrometry** (MS-MS) expts. to be performed on a com. bench-top quadrupole **ion trap mass spectrometer**. Details of the random noise CID expt., the characteristics of the noise spectrum, and the effect of varying noise spectrum and **ion trap** parameters on MS-MS spectra are discussed using N,N-diethylaniline as a model compd. Compromises to the technique imposed by current software flexibility limitations are also discussed. GC-MS-MS spectra, generated using random noise CID, are shown for methamphetamine and amphetamine ionized via isobutane chem. ionization.

**L10 ANSWER 64 OF 76** CA COPYRIGHT 2007 ACS on STN

AN 118:80368 CA

TI Comparison of collisional activation by the boundary effect vs. **tickle excitation** in an **ion trap mass spectrometer**

AU Paradisi, Cristina; Todd, John F. J.; Vettori, Umberto

CS Cent. STud. Mecc. Reaz. Org., CNR, Padua, 35131, Italy

SO *Organic Mass Spectrometry* (1992), 27(11), 1210-15

AB Collisional activation in an **ion trap mass spectrometer** can be achieved by storing parent ions within a narrow zone extending close to the theor. boundaries  $\beta_r = 0$  or  $\beta_z = 0$  of the stability diagram. This

procedure can be used for obtaining **collision-induced dissocn.** of selected parent ions without the need to apply a precisely tuned resonant **tickle** potential between the **end-cap** electrodes. In this investigation a comparison was made between the two methods (**tickle** and **boundary**) of activation based on the efficiency of parent-to-daughter conversion and on the relative abundance of daughter ions for a model system (the  $m/z$  91/92 ratio for n-butylbenzene). The data show that, under conditions of max. efficiency, a comparable amt. of internal energy is present in the ions after activation with the two methods. However, with the **tickle** technique it is possible to increase the internal energy of the parent ions even further, although at the expense of the efficiency, whereas in the case of the boundary activation, the conditions for optimum efficiency almost coincide with those for max. activation and a drastic loss of ions follows any attempt to overcome these limits. It is also found that at any given  $qz$  value used for storing and activating parent ions the permitted mass difference between parent and fragment ions is greater with boundary than with **tickle excitation**.

=> log y

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